Fluid Dynamics in the Multi-Walled Carbon Nanotube

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Multi-walled hollow carbon nanotubes (MWCN) possess extremely high mechanical strength, which, when combined with their ability to provide a conduit for fluid transport at near-molecular length scales, makes them attractive candidates for implementation in future micro- or nanofluidic devices. Therefore, understanding fluid behavior in nanochannels is important for the proper design and efficient operation of such devices. A natural complication underlying the study of fluid dynamics in the CN is the underlying fundamental question of whether fluids behave as continua at these ultrafine length scales, typically down to a nanometer or less.

In the present report the internal pressure and density profile of water, located in the MWCN (an outer diameter of about 100 nm), were calculated in the wide interval of the variation in the thermodynamic variables, including critical point. This was accomplished by solving the isoperimetrical problem about the minimization of free energy of the system in the limited volume under the condition of the constancy of the number of particles. It was found that far from the critical point a substantial change in the density occurs only in the wall layer, whereas near the critical point a significant change of the density in entire volume of system takes place. It is shown that during the calculation of the pressure of water in the CN it is necessary to consider the Tolman correction. The obtained theoretical results are in a good agreement with fluid experiments in the hydrothermal MWCN [1].

References

[1] C.M. Megaridis, A. Guvenc-Yazicioglu, J.A. Libera, Y. Gogotsi. Phys. of Fluids, 14, L5 (2002).